

GAUSSIAN APPROXIMATION POTENTIAL (GAP)

Gaussian Approximation Potential (GAP) is a novel atomistic modelling technique that combines accuracy with speed. By inferring the energy of an atom from the position and identity of its neighbours using a precomputed database of exact quantum mechanical solutions, the potential energy surface of a system of atoms and molecules is approximated. This methodology allows a controllable compromise to be made between the accuracy of Quantum Chemistry models and the speed of Interatomic Potential methods, with applications in a diverse range of fields including pharmaceuticals, aerospace, electronics and biotechnology.

Key benefits of this technology:

- High speed atomistic modelling ($\times 10^6$ compared with DFT for 200 metal atoms)
- Potential Energy Surface directly derived from quantum models
- Controllable accuracy comparable to quantum techniques
- Dynamic updating of modelling accuracy
- Bridges the gap in the atomistic modelling market between quantum and empirical

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Background

Computer modelling of material processes, increasingly on the atomic scale, can help manufacturers to understand the fundamental material mechanisms that underlie the operation of their technology or manufacturing process, and thereby achieve improved product performance.

Traditionally, a choice must be made between (a) highly accurate but slow quantum mechanical modelling and (b) interatomic potential techniques providing speed but with limited accuracy. Gaussian Approximation Potential (GAP) allows accuracy comparable to the former to be combined with the speed of the latter.

Technology

GAP uses a Bayesian probabilistic interpolation algorithm to interpolate a database that is generated a priori using the quantum mechanical potential energy function. Therefore, instead of continually running quantum mechanical models, the user need only build the database once.

A major benefit of this approach is that because it is based on strict mathematical principles of probabilistic inference, the model indicates the accuracy of the interpolation. Thus the GAP technique allows higher accuracy to be achieved by a straightforward expansion of the original database. This process can be automated.

The GAP code allows a database to be built from quantum mechanical data for a wide range of materials, which can then be interrogated to produce a high accuracy potential. Hand-built databases have been created as exemplars and are able to predict complex phenomena with quantum mechanical accuracy for the first time. Ongoing work on each of these exemplars will result in fully general interatomic potentials.

The code comprises two parts: training and prediction. The training is highly automated with very few external parameters.

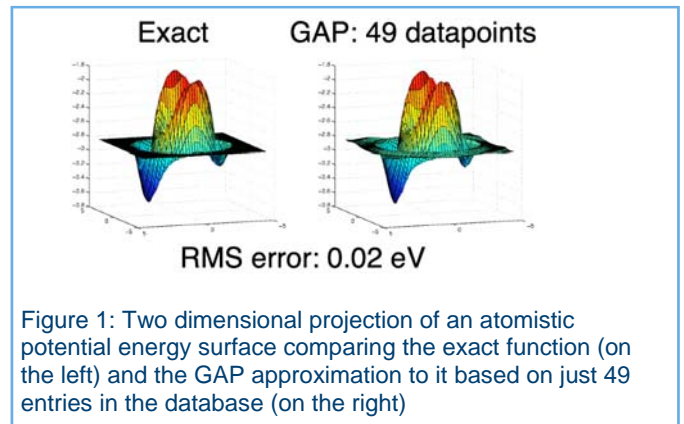


Figure 1: Two dimensional projection of an atomistic potential energy surface comparing the exact function (on the left) and the GAP approximation to it based on just 49 entries in the database (on the right)

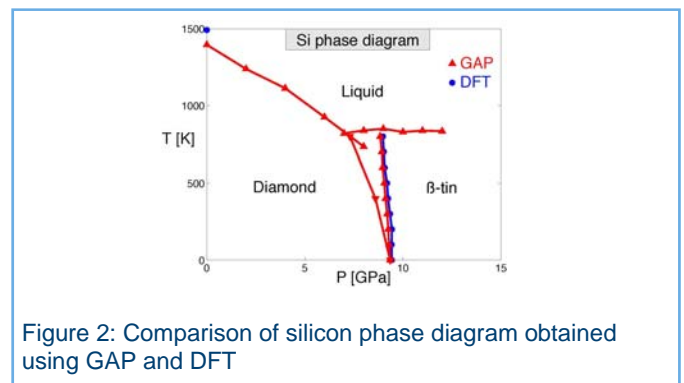


Figure 2: Comparison of silicon phase diagram obtained using GAP and DFT

Table 1: Predictions for various materials

Material	Database Capabilities
Silicon	full P-T phase diagram, amorphous phase transitions, crack propagation
Carbon	phonon dispersion, diamond/graphite transition, thermal expansion, growth of amorphous carbon films
Tungsten	bcc screw dislocation structure
SiO ₂ , TiO ₂	full tensorial elastic properties
Water	dimer interaction energy at the MP2 level to 1 mH accuracy

Commercialisation

We are seeking commercial partners for collaboration, development and licensing of this technology, which is protected by international patent applications.